



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:57 pm BST

PDB ID : 1XSM
Title : PROTEIN R2 OF RIBONUCLEOTIDE REDUCTASE FROM MOUSE
Authors : Kauppi, B.; Nielsen, B.N.; Ramaswamy, S.; Kjoller-Larsen, I.; Thelander, M.;
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Deposited on : 1996-07-03
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

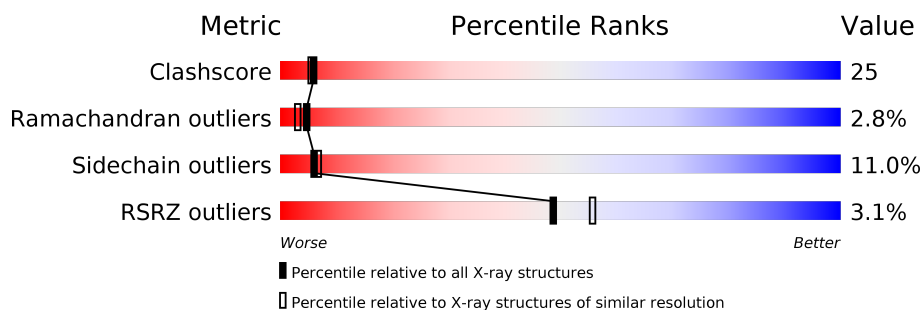
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	390	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2467 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RIBONUCLEOTIDE REDUCTASE R2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2376	1540	394	427	15			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	90	Total	O	0	0
			90	90		

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Chain A:

29% 39% 25% 8% 26%

Amino Acid	Percentage
MET	29%
LEU	39%
SER	25%
VAL	8%
ARG	26%
THR	
PRO	
LEU	
ALA	
THR	
ILE	
ALA	
ASP	
GLN	
GLY	
GLN	
LEU	
GLN	
LEU	
SER	
PRO	
LEU	
LYS	
ARG	
THR	
LEU	
THR	
ALA	
ASP	
LYS	
GLU	
ASN	
THR	
PRO	
PRO	
THR	
LEU	
SER	
SER	
THR	
LYS	
VAL	
LEU	
ALA	
LYS	
SER	
THR	
ALA	
ARG	
ARG	
PHE	
GLN	
ASP	
SER	
ALA	
GLU	
GLY	
SER	

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	77.08 Å 108.93 Å 92.90 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30 29.80 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.9 (25.00-2.30) 96.5 (29.80-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.79 (at 2.31 Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.191 , 0.250 0.186 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 93.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2467	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.33	20/2438 (0.8%)	1.61	42/3293 (1.3%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	GLU	CD-OE1	8.13	1.34	1.25
1	A	287	GLU	CD-OE2	7.38	1.33	1.25
1	A	148	GLU	CD-OE2	7.08	1.33	1.25
1	A	303	GLU	CD-OE1	6.93	1.33	1.25
1	A	153	GLU	CD-OE2	6.71	1.33	1.25
1	A	345	GLU	CD-OE2	6.55	1.32	1.25
1	A	307	GLU	CD-OE2	6.51	1.32	1.25
1	A	224	GLU	CD-OE2	6.33	1.32	1.25
1	A	118	GLU	CD-OE2	6.24	1.32	1.25
1	A	69	GLU	CD-OE1	6.13	1.32	1.25
1	A	261	GLU	CD-OE1	6.05	1.32	1.25
1	A	267	GLU	CD-OE2	6.03	1.32	1.25
1	A	192	GLU	CD-OE2	5.92	1.32	1.25
1	A	343	ARG	NE-CZ	5.77	1.40	1.33
1	A	301	GLU	CD-OE2	5.70	1.31	1.25
1	A	124	GLU	CD-OE1	5.56	1.31	1.25
1	A	326	GLU	CD-OE2	5.44	1.31	1.25
1	A	87	GLU	CD-OE2	5.36	1.31	1.25
1	A	158	GLU	CD-OE2	5.34	1.31	1.25
1	A	121	LYS	C-N	-5.33	1.24	1.34

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	ARG	NE-CZ-NH2	-16.05	112.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	ARG	NE-CZ-NH1	15.90	128.25	120.30
1	A	343	ARG	NE-CZ-NH1	11.37	125.98	120.30
1	A	266	ASP	CB-CG-OD2	-8.47	110.67	118.30
1	A	182	ASP	CB-CG-OD2	-8.35	110.78	118.30
1	A	182	ASP	CB-CG-OD1	8.23	125.71	118.30
1	A	113	ASP	CB-CG-OD2	-7.89	111.19	118.30
1	A	324	TYR	CB-CG-CD1	-7.71	116.37	121.00
1	A	79	ARG	NE-CZ-NH2	7.62	124.11	120.30
1	A	330	ASP	CB-CG-OD1	7.59	125.13	118.30
1	A	187	ASP	C-N-CD	-7.51	104.08	120.60
1	A	139	ASP	CB-CG-OD2	-7.50	111.55	118.30
1	A	225	ARG	CD-NE-CZ	7.41	133.97	123.60
1	A	272	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	A	80	ARG	NE-CZ-NH2	7.11	123.85	120.30
1	A	77	ASN	O-C-N	-7.06	107.69	121.10
1	A	81	PHE	O-C-N	7.05	133.98	122.70
1	A	330	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	A	149	ARG	NE-CZ-NH2	6.91	123.76	120.30
1	A	272	ASP	CB-CG-OD1	6.91	124.52	118.30
1	A	75	ARG	NE-CZ-NH2	6.75	123.68	120.30
1	A	266	ASP	CB-CG-OD1	6.74	124.37	118.30
1	A	191	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	A	139	ASP	CB-CG-OD1	6.62	124.26	118.30
1	A	209	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	A	123	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	A	77	ASN	CA-C-N	6.00	133.91	117.10
1	A	201	MET	CG-SD-CE	5.93	109.69	100.20
1	A	213	ARG	NE-CZ-NH2	5.89	123.24	120.30
1	A	265	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	70	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	A	70	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	90	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	90	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	A	169	MET	CG-SD-CE	5.29	108.67	100.20
1	A	226	VAL	CG1-CB-CG2	-5.28	102.45	110.90
1	A	125	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	143	ASN	CB-CA-C	-5.20	100.00	110.40
1	A	177	TYR	CB-CG-CD1	-5.18	117.89	121.00
1	A	81	PHE	CA-C-N	-5.16	105.85	117.20
1	A	123	ASP	CB-CG-OD1	5.04	122.83	118.30
1	A	324	TYR	CB-CG-CD2	5.02	124.01	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2376	0	2324	117	1
2	A	1	0	0	0	0
3	A	90	0	0	5	1
All	All	2467	0	2324	117	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (117) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:TRP:HD1	1:A:314:ILE:HD12	1.27	0.97
1:A:197:ALA:HA	1:A:201:MET:HG3	1.53	0.90
1:A:246:TRP:CD1	1:A:314:ILE:HD12	2.05	0.90
1:A:120:LEU:HD23	1:A:125:ARG:HG2	1.56	0.88
1:A:201:MET:HB2	1:A:204:VAL:HG12	1.59	0.84
1:A:201:MET:HB2	1:A:204:VAL:CG1	2.08	0.84
1:A:219:GLU:HG2	1:A:219:GLU:O	1.75	0.83
1:A:79:ARG:HG2	1:A:79:ARG:O	1.77	0.83
1:A:222:TYR:O	1:A:226:VAL:HG23	1.81	0.80
1:A:239:GLY:HA3	1:A:305:LEU:HD11	1.63	0.80
1:A:187:ASP:OD1	1:A:188:PRO:HD2	1.85	0.77
1:A:219:GLU:O	1:A:219:GLU:CG	2.32	0.77
1:A:187:ASP:OD2	1:A:189:LYS:HB3	1.86	0.75
1:A:188:PRO:HA	1:A:191:ARG:HD2	1.68	0.75
1:A:144:GLU:O	1:A:148:GLU:HG2	1.87	0.74
1:A:78:PRO:HB2	1:A:80:ARG:HB2	1.71	0.72
1:A:176:MET:HA	1:A:176:MET:HE3	1.70	0.72
1:A:213:ARG:HD2	3:A:858:HOH:O	1.88	0.72
1:A:239:GLY:HA3	1:A:305:LEU:CD1	2.22	0.68
1:A:120:LEU:HD23	1:A:125:ARG:CG	2.23	0.68
1:A:197:ALA:CA	1:A:201:MET:HG3	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:TRP:CE2	1:A:125:ARG:HD3	2.31	0.65
1:A:80:ARG:O	1:A:81:PHE:CB	2.44	0.64
1:A:115:GLN:O	1:A:118:GLU:HB2	1.98	0.63
1:A:325:ILE:N	1:A:325:ILE:HD13	2.13	0.63
1:A:200:THR:O	1:A:202:PRO:HD3	1.99	0.63
1:A:187:ASP:HB3	1:A:190:GLU:OE1	1.97	0.63
1:A:116:HIS:O	1:A:117:TRP:C	2.31	0.62
1:A:197:ALA:HB1	1:A:204:VAL:HG11	1.80	0.62
1:A:205:LYS:HG2	1:A:209:ASP:OD2	1.99	0.62
1:A:77:ASN:O	1:A:78:PRO:C	2.35	0.62
1:A:78:PRO:HG3	1:A:155:GLN:O	2.00	0.61
1:A:120:LEU:HG	1:A:124:GLU:HB2	1.83	0.61
1:A:284:LYS:HB2	1:A:285:PRO:HD2	1.81	0.60
1:A:84:PHE:O	1:A:86:ILE:N	2.35	0.60
1:A:143:ASN:ND2	1:A:170:GLU:HB2	2.17	0.60
1:A:110:LEU:HD11	1:A:180:LEU:HD13	1.85	0.58
1:A:176:MET:HA	1:A:176:MET:CE	2.34	0.58
1:A:149:ARG:NH2	1:A:217:ASP:O	2.37	0.57
1:A:145:ASN:O	1:A:149:ARG:HB2	2.05	0.57
1:A:206:LYS:NZ	1:A:303:GLU:OE2	2.38	0.57
1:A:75:ARG:O	1:A:77:ASN:N	2.38	0.57
1:A:74:LEU:O	1:A:75:ARG:C	2.42	0.56
1:A:134:PHE:CE1	1:A:207:LYS:HD2	2.39	0.56
1:A:265:ARG:O	1:A:265:ARG:HG2	2.04	0.56
1:A:291:ARG:O	1:A:295:THR:HB	2.05	0.56
1:A:109:ASP:OD1	1:A:111:SER:HB2	2.06	0.56
1:A:83:VAL:HG13	1:A:83:VAL:O	2.05	0.55
1:A:78:PRO:HB2	1:A:80:ARG:CB	2.36	0.55
1:A:197:ALA:CB	1:A:201:MET:HG3	2.36	0.55
1:A:136:ALA:HB3	3:A:818:HOH:O	2.05	0.55
1:A:79:ARG:O	1:A:79:ARG:CG	2.51	0.55
1:A:188:PRO:HA	1:A:191:ARG:HB2	1.88	0.55
1:A:260:ASN:N	3:A:821:HOH:O	2.39	0.55
1:A:124:GLU:O	1:A:128:ILE:HG13	2.07	0.54
1:A:80:ARG:O	1:A:81:PHE:HB3	2.08	0.54
1:A:78:PRO:HD3	1:A:155:GLN:HB3	1.90	0.54
1:A:187:ASP:O	1:A:189:LYS:N	2.41	0.54
1:A:78:PRO:CB	1:A:80:ARG:HB2	2.37	0.54
1:A:86:ILE:HG22	1:A:86:ILE:O	2.07	0.54
1:A:196:ASN:HD22	1:A:200:THR:HG23	1.73	0.53
1:A:196:ASN:ND2	1:A:199:GLU:HB2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:GLU:O	1:A:291:ARG:HG3	2.09	0.53
1:A:121:LYS:HB3	1:A:122:PRO:HD2	1.90	0.52
1:A:321:MET:CE	1:A:325:ILE:HD11	2.39	0.52
1:A:122:PRO:O	1:A:125:ARG:N	2.42	0.52
1:A:74:LEU:O	1:A:76:GLU:N	2.43	0.52
1:A:201:MET:CB	1:A:204:VAL:HG12	2.36	0.51
1:A:166:GLN:HB2	3:A:808:HOH:O	2.10	0.50
1:A:114:ILE:CG2	1:A:115:GLN:N	2.74	0.50
1:A:185:ILE:N	1:A:185:ILE:CD1	2.75	0.50
1:A:190:GLU:O	1:A:191:ARG:C	2.49	0.50
1:A:114:ILE:HG23	1:A:115:GLN:N	2.26	0.49
1:A:184:TYR:C	1:A:185:ILE:HD12	2.32	0.49
1:A:205:LYS:CG	1:A:209:ASP:OD2	2.60	0.49
1:A:86:ILE:HD11	1:A:92:TRP:CE2	2.47	0.49
1:A:310:PRO:O	1:A:313:LEU:HD12	2.13	0.49
1:A:110:LEU:HD11	1:A:180:LEU:CD1	2.43	0.48
1:A:239:GLY:HA2	1:A:321:MET:HE1	1.95	0.48
1:A:203:CYS:HB2	1:A:308:ALA:HB1	1.95	0.47
1:A:70:ASP:O	1:A:72:PRO:HD3	2.14	0.47
1:A:343:ARG:HG3	3:A:852:HOH:O	2.15	0.47
1:A:349:ASP:OD1	1:A:349:ASP:N	2.47	0.47
1:A:196:ASN:HD21	1:A:199:GLU:CB	2.28	0.47
1:A:132:LEU:HD23	1:A:132:LEU:HA	1.50	0.47
1:A:190:GLU:O	1:A:193:TYR:N	2.47	0.47
1:A:321:MET:HE1	1:A:325:ILE:HD11	1.96	0.46
1:A:134:PHE:CE1	1:A:207:LYS:CD	2.99	0.46
1:A:196:ASN:O	1:A:200:THR:HG23	2.16	0.45
1:A:200:THR:OG1	1:A:201:MET:N	2.49	0.45
1:A:96:LYS:HE2	1:A:99:GLU:OE1	2.16	0.45
1:A:146:LEU:HD23	1:A:146:LEU:HA	1.73	0.45
1:A:84:PHE:O	1:A:85:PRO:C	2.53	0.45
1:A:78:PRO:C	1:A:80:ARG:N	2.65	0.45
1:A:334:LEU:HD11	1:A:340:LYS:HE3	1.98	0.45
1:A:323:GLN:HG2	1:A:347:PRO:HG3	1.98	0.45
1:A:185:ILE:HD12	1:A:185:ILE:N	2.32	0.45
1:A:176:MET:CE	1:A:176:MET:CA	2.95	0.44
1:A:196:ASN:HD21	1:A:199:GLU:HB2	1.81	0.44
1:A:321:MET:CE	1:A:324:TYR:HD2	2.30	0.44
1:A:109:ASP:OD1	1:A:111:SER:CB	2.65	0.44
1:A:306:THR:HG21	1:A:322:LYS:HE3	1.99	0.44
1:A:321:MET:HE3	1:A:324:TYR:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:LEU:HD23	1:A:305:LEU:HA	1.78	0.43
1:A:116:HIS:H	1:A:116:HIS:CD2	2.37	0.43
1:A:132:LEU:HD13	1:A:180:LEU:HB3	2.00	0.43
1:A:253:MET:HB3	1:A:253:MET:HE2	1.90	0.43
1:A:86:ILE:HD11	1:A:92:TRP:CD2	2.54	0.42
1:A:84:PHE:HD1	1:A:84:PHE:HA	1.46	0.42
1:A:190:GLU:O	1:A:193:TYR:HB3	2.19	0.42
1:A:180:LEU:HA	1:A:180:LEU:HD12	1.90	0.41
1:A:184:TYR:HB2	1:A:185:ILE:HD13	2.02	0.41
1:A:153:GLU:CD	1:A:225:ARG:HH22	2.24	0.41
1:A:78:PRO:CD	1:A:155:GLN:HB3	2.50	0.40
1:A:311:VAL:HB	1:A:316:MET:HB2	2.04	0.40
1:A:321:MET:HE2	1:A:325:ILE:CD1	2.52	0.40
1:A:300:ILE:HD13	1:A:300:ILE:HG21	1.77	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:850:HOH:O	3:A:850:HOH:O[3_756]	1.73	0.47
1:A:121:LYS:NZ	1:A:219:GLU:OE2[8_466]	1.98	0.22

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	286/390 (73%)	260 (91%)	18 (6%)	8 (3%)	5 3

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	GLU

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Mol	Chain	Res	Type
1	A	81	PHE
1	A	113	ASP
1	A	66	PRO
1	A	77	ASN
1	A	119	ALA
1	A	188	PRO
1	A	187	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	254/345 (74%)	226 (89%)	28 (11%)	6 7

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	VAL
1	A	73	LEU
1	A	76	GLU
1	A	80	ARG
1	A	81	PHE
1	A	83	VAL
1	A	84	PHE
1	A	86	ILE
1	A	93	GLN
1	A	113	ASP
1	A	114	ILE
1	A	143	ASN
1	A	176	MET
1	A	179	LEU
1	A	180	LEU
1	A	198	ILE
1	A	201	MET
1	A	203	CYS
1	A	212	LEU

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Mol	Chain	Res	Type
1	A	213	ARG
1	A	253	MET
1	A	281	LEU
1	A	295	THR
1	A	299	ARG
1	A	309	LEU
1	A	319	THR
1	A	331	ARG
1	A	349	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	116	HIS
1	A	126	HIS
1	A	143	ASN
1	A	196	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	288/390 (73%)	-0.35	9 (3%) 49 56	9, 30, 76, 99	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	79	ARG	4.8
1	A	65	ASN	4.5
1	A	77	ASN	4.5
1	A	81	PHE	4.4
1	A	66	PRO	3.7
1	A	76	GLU	3.1
1	A	78	PRO	2.5
1	A	84	PHE	2.3
1	A	199	GLU	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FE	A	401	1/1	0.96	0.11	42,42,42,42	1

6.5 Other polymers ⓘ

There are no such residues in this entry.